# CS 6347

# Lecture 17

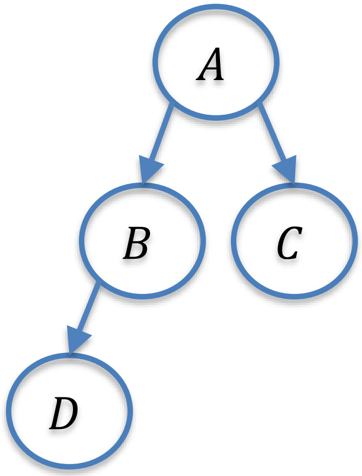
## Introduction to Structure Learning

# Structure Learning

- We have been focusing on parameter learning:
  - E.g., given a graph structure, find the parameters that maximize the log-likelihood
- In practice, the structure of the graph may not be known and may need to be learned from the data
  - For Bayesian networks, we may be only given samples and asked to make predictions

# BN Structure Learning

- Recall that for a fixed Bayesian network  with fully observed data, the MLE of the conditional probability tables was given by the empirical probabilities




| A | B | C | D |
|---|---|---|---|
| 0 | 0 | 1 | 0 |
| 0 | 0 | 1 | 1 |
| 0 | 1 | 0 | 0 |
| 1 | 0 | 0 | 1 |
| 0 | 0 | 1 | 1 |

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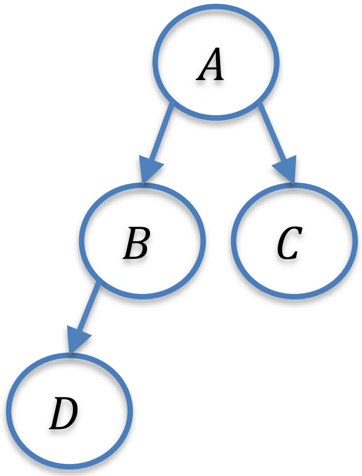


| A | B | C | D |
|---|---|---|---|
| 0 | 0 | 1 | 0 |
| 0 | 0 | 1 | 1 |
| 0 | 1 | 0 | 0 |
| 1 | 0 | 0 | 1 |
| 0 | 0 | 1 | 1 |

| A | P(A) |
|---|---|
| 0 | 4/5 |
| 1 | 1/5 |

| A | B | P(B\|A) |
|---|---|---|
| 0 | 0 | 3/4 |
| 0 | 1 | 1/4 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |

| B | D | P(D\|B) |
|---|---|---|
| 0 | 0 | 1/4 |
| 0 | 1 | 3/4 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |

| A | C | P(C\|A) |
|---|---|---|
| 0 | 0 | 1/4 |
| 0 | 1 | 3/4 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |

# BN Structure Learning

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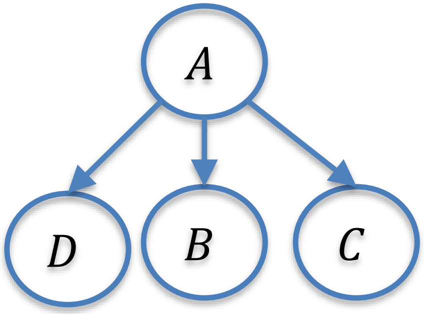



| A | P(A) |
|---|---|
| 0 | 4/5 |
| 1 | 1/5 |

| A | B | P(B\|A) |
|---|---|---|
| 0 | 0 | 3/4 |
| 0 | 1 | 1/4 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |

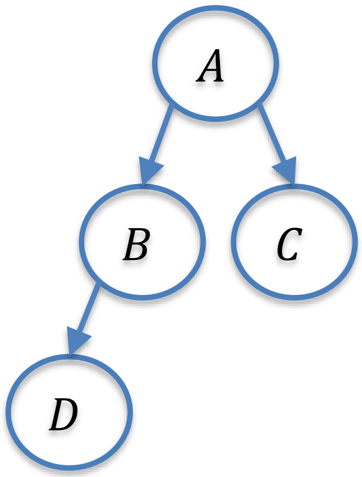
| A | D | P(D\|A) |
|---|---|---|
| 0 | 0 | 1/2 |
| 0 | 1 | 1/2 |
| 1 | 0 | 0 |
| 1 | 1 | 1 |

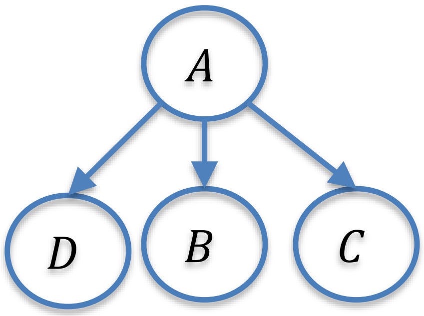
| A | C | P(C\|A) |
|---|---|---|
| 0 | 0 | 1/4 |
| 0 | 1 | 3/4 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |

| A | B | C | D |
|---|---|---|---|
| 0 | 0 | 1 | 0 |
| 0 | 0 | 1 | 1 |
| 0 | 1 | 0 | 0 |
| 1 | 0 | 0 | 1 |
| 0 | 0 | 1 | 1 |

# BN Structure Learning

- Which model should be preferred?



# BN Structure Learning

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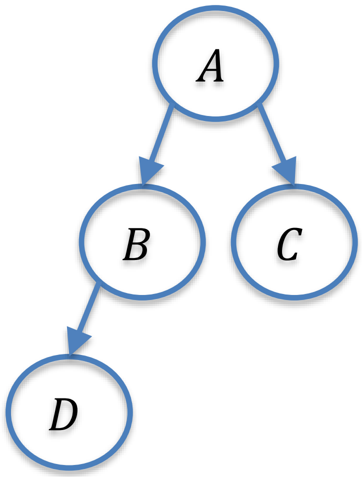
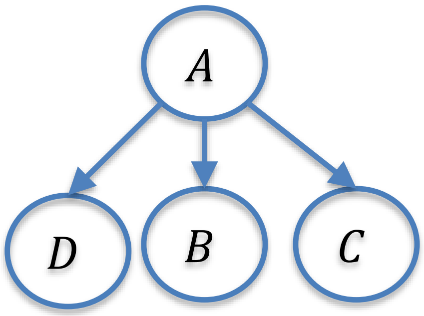
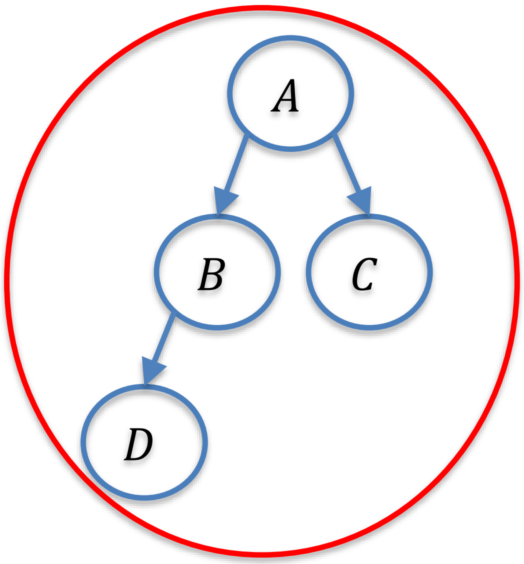


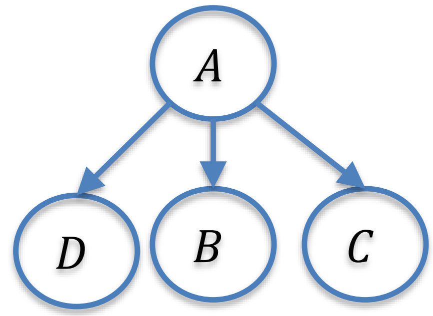




Which one has the highest log-likelihood given the data?

# BN Structure Learning

- Which model should be preferred?




Which one has the highest log-likelihood given the data?

# BN Structure Learning

- Determining the structure that maximizes the log-likelihood is not too difficult
  - A complete DAG always maximizes the log-likelihood
  - This almost certainly results in overfitting
- Alternative is to attempt to learn simple structures
  - Approach 1: Optimize the log-likelihood over simple graphs
  - Approach 2: Add a penalty term to the log-likelihood

# Adding Edges Increases the MLE


Let $p'$ be the empirical probability distribution

$$\frac{\ell_2 - \ell_1}{M} = \frac{1}{M}\sum_m \log \frac{p'(x_D^m | x_B^m, x_C^m)}{p'(x_D^m | x_B^m)}$$

$$= \sum_x p'(x_B, x_C, x_D) \log \frac{p'(x_D | x_B, x_C)}{p'(x_D | x_B)}$$

$$= \sum_x p'(x_B, x_C, x_D) \log \frac{p'(x_B, x_C, x_D)}{p'(x_C | x_B) p'(x_D | x_B) p'(x_B)}$$

$$= d\big(p'(x_B, x_C, x_D) || p'(x_C | x_B) p'(x_D | x_B) p'(x_B)\big) \geq 0$$

# Chow-Liu Trees

- Suppose that we want to find the best tree-structured BN that represents a given joint probability distribution
  - Find the tree-structured BN that maximizes the likelihood
- Let's consider the log-likelihood of a fixed tree $T$
  - Assume that the edges are directed so that each node has exactly one parent

# Chow-Liu Trees

For a fixed tree:

$$\max_{\theta} \log l(\theta, T) = \sum_{i \in V(T)} \sum_{x_{\text{parent}(i)}} \sum_{x_i} \mathrm{N}_{x_{\mathrm{i}}, x_{\text{parent}(i)}} \log \frac{\mathrm{N}_{x_i, x_{\text{parent}(i)}}}{N_{x_{\text{parent}(i)}}}$$

$$= \sum_{i \in V(T)} \left[ \sum_{x_i} N_{x_i} \log N_{x_i} + \sum_{x_{\text{parent}(i)}} \sum_{x_i} \mathrm{N}_{x_{\mathrm{i}}, x_{\text{parent(i)}}} \log \frac{\mathrm{N}_{x_i, x_{\text{parent}(i)}}}{N_{x_i} N_{x_{\text{parent}(i)}}} \right]$$

$$= \left[ \sum_{i \in V} \sum_{x_i} N_{x_i} \log N_{x_i} \right] + \left[ \sum_{(i,j) \in E(T)} \sum_{x_i, x_j} \mathrm{N}_{x_{\mathrm{i}}, x_j} \log \frac{\mathrm{N}_{x_{\mathrm{i}}, x_j}}{N_{x_i} N_{x_j}} \right]$$

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Doesn’t depend on the selected tree!

# Chow-Liu Trees

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$$\max_{\theta} \log l(\theta, T) = \sum_{i \in V(T)} \sum_{x_{\text{parent}(i)}} \sum_{x_i} \mathrm{N}_{x_i, x_{\text{parent}(i)}} \log \frac{\mathrm{N}_{x_i, x_{\text{parent}(i)}}}{N_{x_{\text{parent}(i)}}}$$

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$$= \left[ \sum_{i \in V} \sum_{x_i} N_{x_i} \log N_{x_i} \right] + \left[ \sum_{(i,j) \in E(T)} \sum_{x_i, x_j} \mathrm{N}_{x_i, x_j} \log \frac{\mathrm{N}_{x_i, x_j}}{N_{x_i} N_{x_j}} \right]$$

This is the (empirical) **mutual information**, usually denoted $I(x_i; x_j)$

# Chow-Liu Trees

- **To maximize the log-likelihood, it then suffices to choose the tree $T$ that maximizes**

$$\max_T \sum_{i,j} I(x_i; x_j)$$

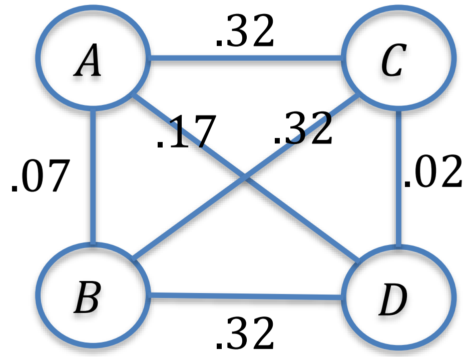
- This problem can be solved by finding the maximum weight spanning tree in the complete graph with edge weight $w_{ij}$ given by the mutual information over the edge $(i, j)$
  - Greedy algorithm works: at each step, pick the largest remaining edge that does not form a cycle when added to the already selected edges

# Chow-Liu Trees

- To use this technique for learning, we simply compute the mutual information for each edge using the empirical probability distributions and then find the max-weight spanning tree

- As a result, we can learn tree-structured BNs in polynomial time
  - Can we generalize this to all DAGs?

# Chow-Liu Trees: Example




- Edge weights correspond to empirical mutual information for the earlier samples

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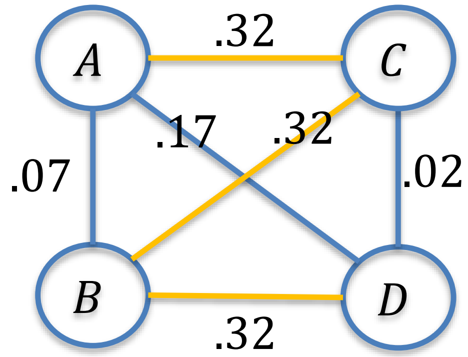


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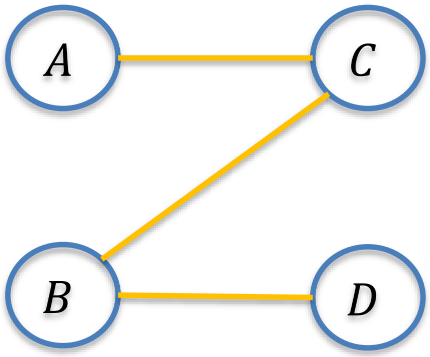


- Any directed tree (where each node has one parent) over these edges maximizes the log-likelihood
  - Why doesn't the direction matter?

# Approach 2: Penalized Likelihood

- Add a penalty term to the log-likelihood that can depend on the number of samples and the chosen structure

$$\ell(G,\theta) = \sum_m \log p_G(x^m|\theta) - \eta(M)Dim(G)$$

- $\eta(M)$ is only a function of the number of samples
  - $\eta(M) = constant$ called the Akaike information criterion
  - $\eta(M) = \frac{\log(M)}{2}$ called the Bayesian information criterion
- $Dim(G)$ is the number of parameters needed to represent $G$